Journal of Molecular Structure (Theochem), 226 (1991) 365
Elsevier Science Publishers B.V., Amsterdam

AUTHOR INDEX

Avnir, D. 211

Baptist, S. 99
Bartha, F. 351
Birner, P. 223
Bogár, F. 351

Ciuffo, G.M. 327

Daudel, R. 351
De Alti, G. 265
Decleva, P. 265

Edgecombe, K.E. 157
Enriz, R.D. 327

Fernández, B. 181
Fraga, S. 87
Fronzoni, G. 265

Graña, A.M. 303
Grand, A. 251

Hameka, H.F. 241
Hamilton, W. 147
Hanson, L.K. 111
Hodges, R.S. 87
Huhta, D. 99

Jáurégui, E.A. 327

Kapuy, E. 351
Karpfen, A. 223
Khalil, M. 73
Köhler, H.-J. 223
Koulis, M. 1
Kovach, I.M. 99
Kozmutza, C. 351
Krusic, P.J. 251

Leroy, G. 307
Li, W.-K. 285
Lischka, H. 223
Lisini, A. 265
Liu (Liu Fan), F. 197

Mattar, S.M. 147
Mayer, I. 47
Meath, W.J. 1
Meyeer, A.Y. 211

Noodleman, L. 251

Paddon-Row, M.N. 285
Parker, J.M.R. 87

Ríos, M.A. 181, 303
Rodriquez, J. 303

San Fabian, E. 87
Sana, M. 307
Silvi, B. 129
Smith, Jr., V.H. 73
Subra, R. 251
Surjan, P.R. 39, 47
Szalay, P.G. 351

Tapai, O. 59
Thornton, S. 87

Weaver, D.F. 73
Wong, S.S. 285

Zhan, C.-G. 339
Zheng, F. 339

Journal of Molecular Structure (Theochem), 226 (1991) 366–368
Elsevier Science Publishers B.V., Amsterdam

SUBJECT INDEX

Active site interactions
Active site interactions in hydrated trypsin-organophosphate adducts: a YETI molecular mechanics study 99
Alcohols
Theoretical prediction of structures and infrared frequencies. Part II. Alcohols and ethers 241
AlH_4 radical
On the structure and stability of the AlH_4 radical and its potential energy surface for rearrangement and dissociation: an ab initio MO study 285
All-trans conjugated polyenes
The transferability of some molecular properties in all-trans conjugated polyenes 351
AM1 semi-empirical quantum mechanical study
An AM1 semi-empirical quantum mechanical study of the polyhydration of amino acid side chains 73
Amino acid side chains
An AM1 semi-empirical quantum mechanical study of the polyhydration of amino acid side chains 73

Biorthogonal perturbation theory
Intermolecular interactions: biorthogonal perturbation theory revisited 47
Block diagonalization
The canonical orthogonalization of AO basis set and block diagonalization of the Hamiltonian matrix 339

Canonical orthogonalization
The canonical orthogonalization of AO basis set and block diagonalization of the Hamiltonian matrix 339
Charge transfer
Environmentally induced spectral shifts of oxidized lumiflavin: charge transfer and electrochromic effects 111
Chirality measure
Quantifying the degree of molecular shape distortion. A chirality measure 211
Cimetidine
Theoretical study of cimetidine and rigid analogues 327
$Co(CO)_3NO$
Theoretical study of the electronic structure and photoelectron spectra of $Ni(CO)_4$, $Co(CO)_3NO$, $Fe(CO)_2(NO)_2$, $MnCO(NO)_3$ and $Cr(NO)_4$ 265
$Cr(NO)_4$
Theoretical study of the electronic structure and photoelectron spectra of $Ni(CO)_4$, $Co(CO)_3NO$, $Fe(CO)_2(NO)_2$, $MnCO(NO)_3$ and $Cr(NO)_4$ 265

Dissociation
On the structure and stability of the AlH_4 radical and its potential energy surface for rearrangement and dissociation: an ab initio MO study 285

Electrochromic effects
Environmentally induced spectral shifts of oxidized lumiflavin: charge transfer and electrochromic effects 111
Electron density analysis
A topological electron density analysis of tricoordinate phosphorus inversion processes 157
Enthalpies of formation
Theoretical thermochemistry. The enthalpies of formation of some XH_n and XYH_n compounds 307
Ethers
Theoretical prediction of structures and infrared frequencies. Part II. Alcohols and ethers 241
Extremum method
The extremum method in quantum chemistry. Part I. Extremum of $tr(\mathbf{B}^T\mathbf{PC})$ and the trace algebra 197

$Fe(CO)_2(NO)_2$
Theoretical study of the electronic structure and photoelectron spectra of $Ni(CO)_4$,

$Co(CO)_3NO$, $Fe(CO)_2(NO)_2$, $MnCO(NO)_3$ and $Cr(NO)_4$ 265

$Fe(CO)_4^{\pm}$
$Fe(CO)_4^{\pm}$ radical anion: theoretical study of the electronic structure and magnetic properties 251

Geochemistry
Application of quantum chemistry to geochemistry and geophysics 129

Geophysics
Application of quantum chemistry to geochemistry and geophysics 129

Hydroxy-1-indanone
Ab initio study of the structure and tautomerism in 7-hydroxy-1-indanone 303

Infrared frequencies
Theoretical prediction of structures and infrared frequencies. Part II. Alcohols and ethers 241

Intermolecular interactions
On the perturbation operator in ab initio theories of intermolecular interactions 39

Intermolecular potentials
On the construction and use of reliable two- and many-body interatomic and intermolecular potentials 1

LCAO techniques
The ground and some excited state geometries of vanadium monocarbonyl by local-spin-density LCAO techniques 147

Lumiflavin
Environmentally induced spectral shifts of oxidized lumiflavin: charge transfer and electrochromic effects 111

Magnetic properties
$Fe(CO)_4^{\pm}$ radical anion: theoretical study of the electronic structure and magnetic properties 251

$MnCO(NO)_3$
Theoretical study of the electronic structure and photoelectron spectra of $Ni(CO)_4$, $Co(CO)_3NO$, $Fe(CO)_2(NO)_2$, $MnCO(NO)_3$ and $Cr(NO)_4$ 265

$Ni(CO)_4$
Theoretical study of the electronic structure and photoelectron spectra of $Ni(CO)_4$, $Co(CO)_3NO$, $Fe(CO)_2(NO)_2$, $MnCO(NO)_3$ and $Cr(NO)_4$ 265

Perturbation operator
On the perturbation operator in ab initio theories of intermolecular interactions 39

Phosphorus inversion
A topological electron density analysis of tricoordinate phosphorus inversion processes 157

Photoelectron spectra
Theoretical study of the electronic structure and photoelectron spectra of $Ni(CO)_4$, $Co(CO)_3NO$, $Fe(CO)_2(NO)_2$, $MnCO(NO)_3$ and $Cr(NO)_4$ 265

Polyhydration
An AM1 semi-empirical quantum mechanical study of the polyhydration of amino acid side chains 73

Polysulfane series
An ab initio study of the polysulfane series H_2S_2 to H_2S_6 and of S_8 223

Proteins
Theoretical prediction of secondary structures of proteins using recognition factors 87

Proton transfer
An ab initio study of proton transfer in triose reductone 181

Radical anion
$Fe(CO)_4^{\pm}$ radical anion: theoretical study of the electronic structure and magnetic properties 251

Rearrangement
On the structure and stability of the AlH_4 radical and its potential energy surface for rearrangement and dissociation: an ab initio MO study 285

S_8
An ab initio study of the polysulfane series H_2S_2 to H_2S_6 and of S_8 223

Secondary structures
Theoretical prediction of secondary structures of proteins using recognition factors 87

Solvent-effect representation
On the theory of solvent-effect represen-

tation. Part I. A generalized self-consistent reaction field theory 59

Tautomerism
Ab initio study of the structure and tautomerism in 7-hydroxy-1-indanone 303
Trace algebra
The extremum method in quantum chemistry. Part I. Extremum of tr ($\mathbf{B}^{T}\mathbf{PC}$) and the trace algebra 197
Triose reductone
An ab initio study of proton transfer in triose reductone 181
Trypsin-organophosphate adduct
Active site interactions in hydrated trypsin-organophosphate adducts: a YETI molecular mechanics study 99

Vanadium monocarbonyl
The ground and some excited state geometries of vanadium monocarbonyl by local-spin-density LCAO techniques 147

XH_n
Theoretical thermochemistry. The enthalpies of formation of some XH_n and XYH_n compounds 307
XYH_n
Theoretical thermochemistry. The enthalpies of formation of some XH_n and XYH_n compounds 307

YETI molecular mechanics
Active site interactions in hydrated trypsin-organophosphate adducts: a YETI molecular mechanics study 99